1,1,2,2-Tetrachloroethane 79-34-5 | DTXSID7021318

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 8.47 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.85e-01

Confidence level: 6.63e-01

Nearest Neighbors from the Training Set

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2,3-Dimethylbutane Measured: 4.62 Predicted: 313 Image not found

Pentatriacontane Measured: 12.0 Predicted: 8.42e-12 Image not found

Phoxim

Measured: 9.38e-01 Predicted: 1.27e-05

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Cyclohexane Measured: 89.0 Predicted: 91.3 Image not found

1,4-Pentadiene Measured: 97.3 Predicted: 543